Lattice QCD Calculation of the Two-Photon Exchange Contribution to the Muonic-Hydrogen Lamb Shift

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Based on Phys. Rev. Lett. 128 (2022) 17, 172002 + new progress

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PREN & μASTI conference

Outline

1. Background
2. Lattice QCD calculation of TPE to μH Lamb shift
   (based on PRL 128 (2022) 17, 172002 + new progress)
3. Lattice QCD calculation of subtraction function
   (ongoing)
4. Conclusion & Outlook

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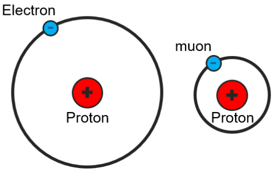
Muonic-hydrogen Lamb shift

- Lamb shift in μH: most precise way to measure proton charge radius.



- m_μ is about 200 times of $m_e \to \mu$H Bohr radius is about 1/200 of H

$\Rightarrow$ much more sensitive to proton structure, especially the charge radius.

- Experiments done in 2010 and 2013, by CREMA at PSI

$$\sqrt{\langle r_p^2 \rangle} = 0.84087(26)_{\text{exp}}(29)_{\text{theo}} \text{ fm}$$

10 times more precise than hydrogen / scattering result.

(Nature 466 (2010) 213, Science 339 (2013) 417)

- Proton structure effects beyond charge radius also enhanced

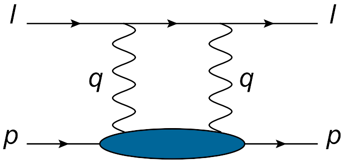
$\Rightarrow$ Major source of theoretical uncertainty.

- Theory for μH Lamb shift (Science 339 (2013) 417. Ann. of Phy. 331 (2013), 127)

Exp. value		Theory
$\Delta E_{\text{2S-2P}}$	$=$	$\Delta E_{\text{structure indep.}} + \Delta E_{\text{proton size}} + \Delta E_{\text{TPE}}$
$202370.6(2.3)$	$=$	$206033.6(1.5) - 5227.5(1.0)\langle r_p^2 \rangle + 33.2(2.0)$

(Units in μeV and fm)

- Two-photon exchange (TPE): the hadronic effect.



- The uncertainty of structure-independent part is further reduced

$$\Delta E_{\text{2S-2P}} = 206034.7(0.3) - 5227.5(1.0)\langle r_p^2 \rangle + 33.2(2.0)$$

Exp. value will also be improved by at least 5 times.

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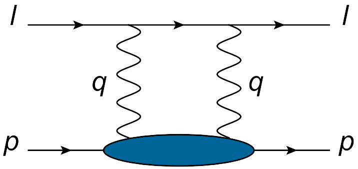
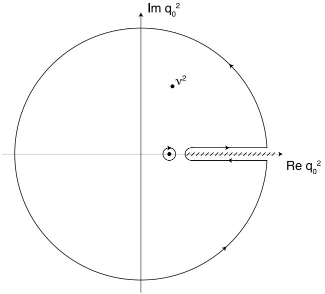
- TPE will dominate the total uncertainty.



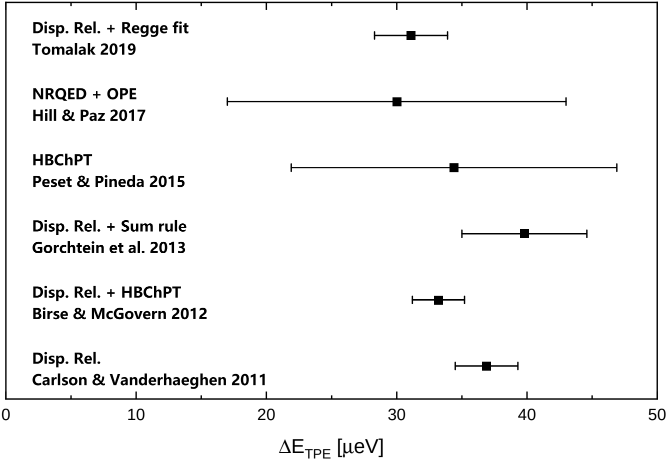


- TPE is sensitive to low-energy structure: non-perturbative QCD
- Dispersion relation: turn scattering data into amplitudes

- Cauchy formula + optical theorem
- No contribution from $\mathcal{C}_\infty$, otherwise a subtraction must be performed
- Unfortunately here we need once-subtracted DR

- Subtraction leads to a "subtraction function": can not be fully extracted from experimental data.

Two-photon exchange



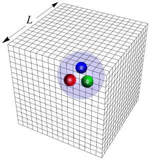
- Previous work: DR and/or EFTs. Results are in good agreement.
- Non-perturbative $\Rightarrow$ lattice QCD

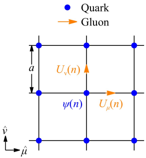
- can calculate full TPE directly
- or calculate the subtraction function, then combined with DR calculation

- Lattice QCD: path integral formalism of QCD in Euclidean space

$$\langle O \rangle = \frac{1}{Z} \int [DU] \, \hat{O} \exp\left\{ \underbrace{-S_g[U]}_{\text{gluon}} + \underbrace{\mathrm{Tr}\ln(M[U])}_{\text{quark}} \right\}$$

$$\Rightarrow \frac{1}{N} \sum_i O_i$$





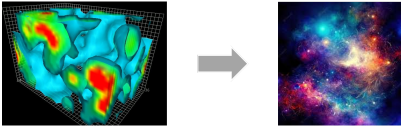
- Dimension of the integral $\propto$ number of points $\sim 10^7$

$\rightarrow$ Monte Carlo method, average over configurations.

- Action is local $\rightarrow$ configurations stored in position space.

- Three limit for LQCD calculation to reach the physical point:

- lattice size $L \rightarrow \infty$
- lattice spacing $a \rightarrow 0$
- quark mass $m_q \rightarrow m_{q,\mathrm{phy}}$ (or pion mass $m_\pi \rightarrow m_{\pi,\mathrm{phy}}$)



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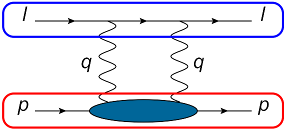
- TPE diagram can be calculated using lattice QCD



Leptonic part $L_{\mu\nu}$ analytically known

Hadronic part $H_{\mu\nu}$ lattice QCD

$$\Delta E^{\text{box}} = \int \frac{\mathrm{d}^4 q}{(2\pi)^4} L_{\mu\nu}(q) H_{\mu\nu}(q) = \int \mathrm{d}^4 x \; L_{\mu\nu}(x) H_{\mu\nu}(x)$$

But: free lepton $\rightarrow$ TPE diagram is IR divergent

- The real definition of IR finite TPE: need to remove

1) point-like proton contribution (form factor $G_E = G_M = 1$)

$$T_1^{\text{pt}} = \frac{M}{\pi} \frac{\nu^2}{Q^4 - 4M^2\nu^2}, \qquad T_2^{\text{pt}} = \frac{M}{\pi} \frac{Q^2}{Q^4 - 4M^2\nu^2}$$

2) charge radius term from third Zemach moment contribution

$$\Delta E^{\text{rad}} = \alpha^2 |\phi_n(0)|^2 \int \frac{\mathrm{d}Q^2}{Q^2} \frac{8mM}{3(M+m)Q} \langle r_p^2 \rangle$$

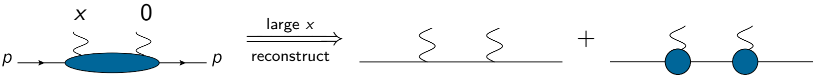
- IR divergence shall cancel analytically even for numerical calculation. How?

- Infinite-volume reconstruction (IVR) method.

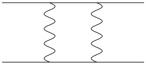
Feng, Jin, PRD 100, 094509 (2019)

- Idea: low-energy structure $\to$ long-distance hadronic function

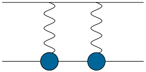
$\Rightarrow$ reconstruct point-like + charge radius



- We thus find the appropriate weight functions L^{pt}, L^{rad}



$$= c^{\mathrm{pt}} \int \mathrm{d}^4x \, L^{\mathrm{pt}}(x) H(x)$$



$$= c^{\mathrm{rad}} \int \mathrm{d}^4x \, L^{\mathrm{rad}}(x) H(x)$$

therefore

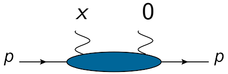
$$\Delta E = \int \mathrm{d}^4x \underbrace{\left[L(x) - c^{\mathrm{pt}} L^{\mathrm{pt}}(x) - c^{\mathrm{rad}} L^{\mathrm{rad}}(x)\right]}_{\text{IR finite}} H(x)$$

$$\equiv \int \mathrm{d}^4x \, L^{\mathrm{sub}}(x) H(x)$$

Weight function $L^{\mathrm{sub}}(x)$ is IR finite $\to$ maintain IR cancellation automatically.

Finite-volume effect & signal-to-noise problem

- Signal-to-noise ratio decays exponentially at long distance:



$$H(x)/\delta H(x) \sim \exp\left\{-\left(M_p - \frac{3}{2}m_\pi\right)|x|\right\}$$

- Weight function $L^{\text{sub}}(\vec{x}, t_s)$ increases rapidly as $|x|$ increases

$\Rightarrow$ Significant finite-volume effect.

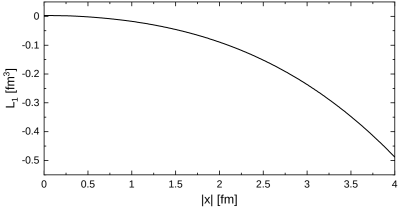


Figure: $L^{\text{sub}}(x)$ increases with $|x|$

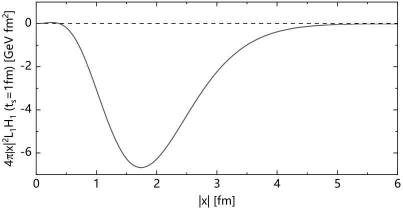


Figure: model estimate: $4\pi|x|^2 L(x)H(x)$

- Converges at $|x| \sim 5$ fm.

$\Rightarrow$ $L \sim 10$ fm lattice box required. Possible, but H(x) will be very noisy.

- Optimized subtraction scheme, idea: $A = (A - B) + B$
- Recall the charge conservation and charge radius

$$1 = \int \mathrm{d}^4x\ L^{\mathrm{pt}}(x)H(x), \quad \langle r_p^2 \rangle = \int \mathrm{d}^4x\ L^{\mathrm{rad}}(x)H(x)$$

We split the TPE correction into

$$\Delta E = \underbrace{(\Delta E - c_0 - c_r \cdot \langle r_p^2 \rangle)}_{\Delta E^{(r)}} + c_0 + c_r \cdot \langle r_p^2 \rangle$$

with $\Delta E^{(r)}$ calculated on lattice using reduced weight function

$$L^{(r)}(x) = L^{\mathrm{sub}}(x) - c_0 L^{\mathrm{pt}}(x) - c_r L^{\mathrm{rad}}(x)$$

- The subtraction coefficients c_0 and c_r are chosen by minimizing

$$I(c_0,\ c_r) = \int_{R_{\mathrm{min}}}^{R_{\mathrm{max}}} \mathrm{d}x\,(4\pi x^2)|L^{(r)}(x)|^2$$

Finite-volume effect & signal-to-noise problem

- Main contribution comes from the range of $1 - 3$ fm

we therefore choose $R_{\text{min}} = 1$ fm and $R_{\text{max}} = 3$ fm to minimize $L^{(r)}(x)$

- Minimization yields

$$\Delta E_{\text{TPE}} = 0.77\ \mu\text{eV} + 93.72 \cdot \langle r_p^2 \rangle\ \mu\text{eV}/\text{fm}^2 - \Delta E_{\text{lat}}$$

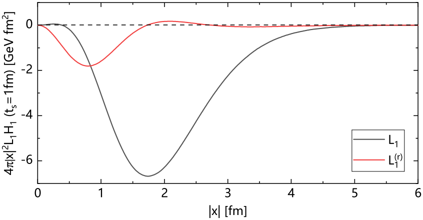


Figure: model estimate for $L_1(x)$ and $L_1^{(r)}(x)$

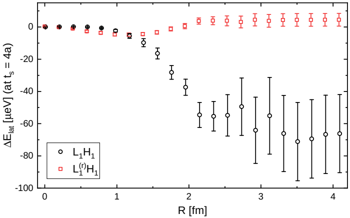


Figure: Numerical partial sum

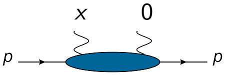
- ΔE_{lat} with reduced weight function

$\Rightarrow$ Finite-volume effect: $L \sim 10$ fm $\rightarrow 5$ fm, with error reduced by ~ 6 times.

Four-point correlation function

- Many LQCD works based on 2pt and 3pt correlation functions

but this work requires nucleon 4pt functions.



- Complexity: 3pt $\to$ 4pt, one more summation over L^3

$\Rightarrow$ increased by $\sim 10^4 - 10^6$, new approach is needed.

- Solved by random field sparsening technique. Detmold et al., PRD 104, 034502 (2021)

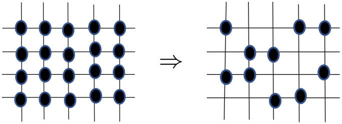
Li, et al., PRD 103, 014514 (2021)

- Sum over full space $\to$ random points.

- Strong correlation between data points

$\Rightarrow$ Number of sums reduced by $10^2 \sim 10^3$,

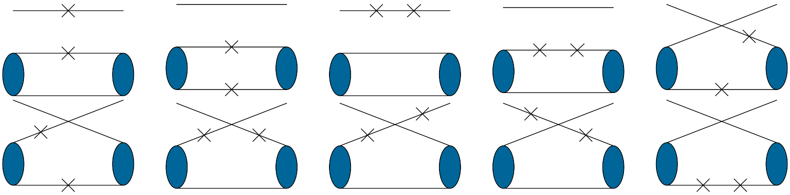
with negligible loss of precision



- Increase in computational complexity becomes acceptable

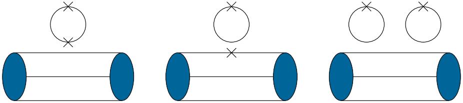
- One more point → more types of quark field contractions.

  - quark connected diagrams (10 types):



  - quark disconnected diagrams (3 types):

notorious for high cost and bad signal-to-noise!



- Our calculation includes all types of connected diagrams and the first type of disconnected diagrams (other two suppressed by flavor SU(3))

Lattice setup

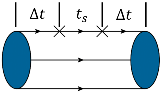
- Gauge ensemble: pion mass near physical

Ensemble	m_π [MeV]	L/a	T/a	a[fm]	N_{conf}
24D	142	24	64	0.1943(8)	131

- Time separation sets for four-point correlation function:

$$\{\Delta t_i/a, \Delta t_f/a\} = \{1,2\},\{2,1\},\{2,2\},\{2,3\},\{3,2\},\{3,3\}$$

$$t_s/a = 2,3,4,5$$



total source-sink time separation ranges from 1.0 to 2.1 fm

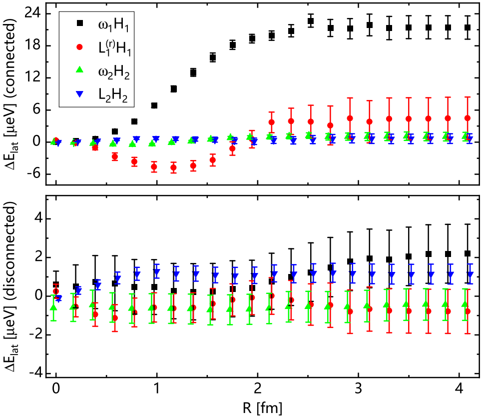
- Published result reuse the point-source propagators already generated in previous calculation → demonstrate the feasibility

⇒ better use the smeared-source propagators → we are currently generating!

Numerical results

- Partial sum $\sum_{|x|<R}$ of the result (at $\{\Delta t_i, \Delta t_f, t_s\} = \{2a, 2a, 4a\}$)

Upper: connected. Lower: disconnected.

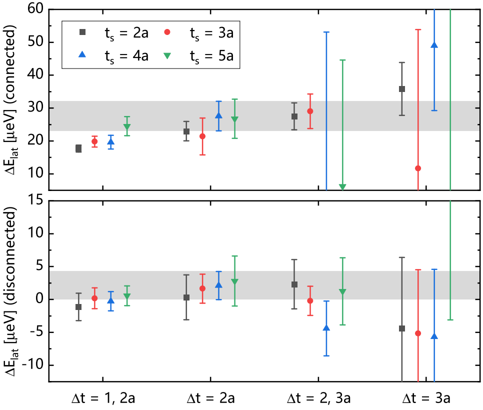


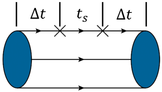
- All contributions converge at $R \sim 2.5$ fm

$\Rightarrow$ Finite-volume effects are well under control within current uncertainties.

- Multiple sets of time separation to confirm ground-state saturation.

Upper: connected. Lower: disconnected.





$$\Delta E_{\text{lat}} = \begin{cases} 27.6(4.5)\ \mu\text{eV}, & \text{connected part,} \\ 2.1(2.1)\ \mu\text{eV}, & \text{disconnected part,} \\ 29.7(4.9)\ \mu\text{eV}, & \text{total contribution.} \end{cases}$$

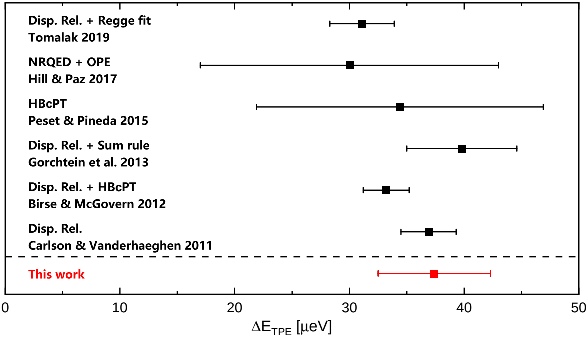
Numerical results

- The total TPE contribution is given by

$$\Delta E_{\text{TPE}} = -28.9(4.9)\ \mu\text{eV} + 93.72\ \mu\text{eV}/\text{fm}^2 \cdot \langle r_p^2 \rangle$$
$$= 37.4(4.9)\ \mu\text{eV}$$

If not using the optimized subtraction scheme, we get $\Delta E_{\text{TPE}} = 40(24)\ \mu\text{eV}$.

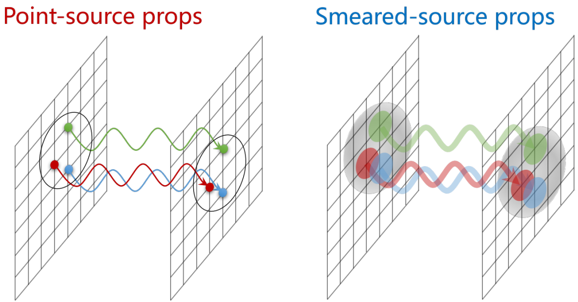
- Compared with previous theoretical work



Next step: more statistics and better control the systematics

Improvements

- Here we highlight the improvements from smeared-source propagators.



- creation operator with correct quantum number can generate proton state

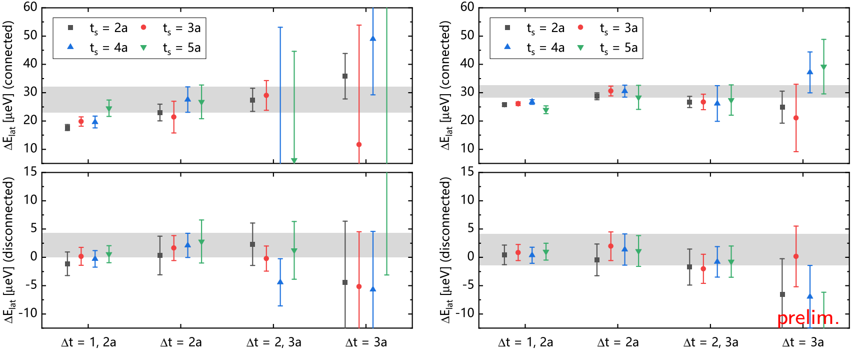
but also generate all possible excited states ⇒ excited-state contamination

- Proton is not a point particle, extend the propagators in a reasonable way

(e.g. Gaussian) can increase the overlap ⇒ smeared-source propagators.

Improvements: smeared propagators

- Point-source props ($n_{conf} \sim 130$) $\rightarrow$ smeared-source props ($n_{conf} \sim 110$)
  still generating!



- Excited-state contamination better controlled
- Statistical uncertainty for connected part reduced by $\sim 50\%$

$\rightarrow$ smeared props are more correlated, field sparsening works more efficiently

More statistics & more ensembles are ongoing – stay tuned for that!

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Subtraction function

- Another way: evaluate the subtraction function with lattice QCD.

Motivation: DR + LQCD could be more precise compared to full LQCD

- F. Hagelstein & V. Pascalutsa suggest performing the subtraction at

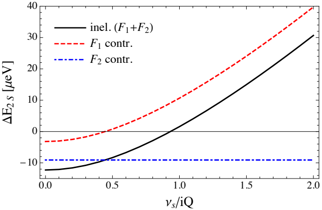
$(\nu_s, Q^2) = (iQ, Q^2)$ rather than $(0, Q^2)$.

Nucl. Phys. A 1016 (2021) 122323

$\Delta E^{(\text{inel})}_{\text{TPE}}(\nu_s = iQ) = 1.6\ \mu\text{eV}$ vs

$\Delta E^{(\text{inel})}_{\text{TPE}}(\nu_s = 0) = -12.3\ \mu\text{eV}$

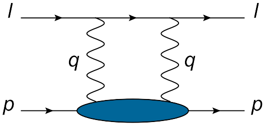
$\Rightarrow$ inelastic term is suppressed



- Situation for joint calculation:

- DR calculation: dominated by elastic term and is very precise
- LQCD calculation: this point can be accessed by simply set $Q = (Q, \vec{0})$

Dispersion relation



- In more detail

Blob: doubly-virtual Compton scattering (VVCS)

$$T_{\mu\nu} = \left(-\delta_{\mu\nu} + \frac{Q_\mu Q_\nu}{Q^2}\right) T_1(\nu, Q^2) - \left(P_\mu - \frac{P\cdot Q}{Q^2} Q_\mu\right)\left(P_\nu - \frac{P\cdot Q}{Q^2} Q_\nu\right) \frac{T_2(\nu, Q^2)}{M^2}$$

- $T_{1,\,2}(\nu, Q^2)$ can be reconstructed via dispersion relations.

but once subtraction is needed for $T_1(\nu, Q^2)$

- Two ways to perform the subtracted DR:

1) Separate the Born term first, then perform DR to the non-Born part

$$\begin{aligned} T_1(\nu, Q^2) &= T_1^{\text{Born}}(\nu, Q^2) + T_1^{\text{non-Born}}(\nu, Q^2) \\ &= T_1^{\text{Born}}(\nu, Q^2) + T_1^{\text{inel}}(\nu, Q^2) + T_1^{\text{non-Born}}(iQ, Q^2) \end{aligned}$$

2) Perform DR directly to full amplitude

$$T_1(\nu, Q^2) = T_1^{\text{el}}(\nu, Q^2) + T_1^{\text{inel}}(\nu, Q^2) + T_1(iQ, Q^2)$$

Lattice QCD calculation of subtraction function

- For LQCD, we prefer calculate $T_1(iQ, Q^2)$ instead of $T_1^{\text{non-Born}}(iQ, Q^2)$.

- we can only simulate the full hadronic function $H_{\mu\nu}(x)$, not $H_{\mu\nu}^{\text{non-Born}}(x)$.

- To avoid IR divergence, we subtract the contribution from $\lim_{Q\to 0} T_1(iQ, Q^2)$

then add it back to the elastic part.

- The size of each part is estimated below

Subt. point	ΔE^{el}	ΔE^{inel}	ΔE^{subt} [μeV]	subt. from LQCD
$\nu_s = iQ$	27.5	-1.6	$\lesssim 10$	uncertainty $< 20\%$ is OK
$\nu_s = 0$	-15.9	12.3	~ 30	not favored

Elastic: using dipole form factors with $\sqrt{r_E^2} = \sqrt{r_M^2} = 0.85$ fm

Inelastic: Christy-Bosted parameterization

Subtraction: assuming total $\Delta E_{\text{TPE}} \sim 30$ μeV

$\Rightarrow$ Conclusion: lattice calculation also favors $(\nu_s, Q^2) = (iQ, Q^2)$

Lattice QCD calculation of subtraction function

- Need to extract $T_1(iQ, Q^2)$ from $T_{\mu\nu}$ (or $H_{\mu\nu}(x)$, simulated by lattice)

$$T_{\mu\nu} = \left(-\delta_{\mu\nu} + \frac{Q_\mu Q_\nu}{Q^2}\right) T_1(\nu, Q^2) - \left(P_\mu - \frac{P \cdot Q}{Q^2} Q_\mu\right)\left(P_\nu - \frac{P \cdot Q}{Q^2} Q_\nu\right) \frac{T_2(\nu, Q^2)}{M^2}$$

at $\vec{Q} = \vec{0}$ non diagonal elements vanish $\rightarrow$ one can use either $\sum_i T_{ii}$ or T_{00}

- For simplicity, we define ξ as $\nu = i\xi Q$

for $\sum_i T_{ii}$ it is straightforward, we get

$$T_1(iQ, Q^2) = -\frac{1}{3}\sum_i T_{ii}\Big|_{\xi=1}$$

for T_{00}, it vanishes at $\xi = 1$, but the "derivative" survives

$$T_1(iQ, Q^2) = -\lim_{\xi \to 1} \frac{1}{1-\xi^2} T_{00}\Big|_{\xi}$$

both can be used, but on lattice they have different syst. and stat. error.

- We find it's better to extract subtraction function from T_{00}

- current conservation better held and smaller statistical uncertainty.

- Evaluate the integral for TPE to Lamb shift, we get

$$\Delta E^{\text{subt}} = 16\pi\alpha^2|\phi_n(0)|^2 \int \mathrm{d}Q \underbrace{\left(-\frac{\gamma(\tau_l)}{Q^2}[T_1(iQ,Q^2) - \lim_{Q\to 0} T_1(iQ,Q^2)]\right)}_{f(Q)}$$

with $\tau_l = Q^2/(4m_\mu^2)$ and $\gamma(\tau) = (1-2\tau)[(1+\tau)^{1/2} - \tau^{1/2}] + \tau^{1/2}$

- The weight function is monotonically falling and

$$\gamma(\tau_l) = \begin{cases} 1, & Q \to 0 \\ \dfrac{3m_\mu}{2Q}, & Q \to \infty \end{cases}$$

the contribution is heavily weighted to small momentum.

- For zero-momentum limit, the low-energy expansion gives

$$f(0) = \frac{\alpha_E}{4\pi\alpha_{\text{EM}}} - \frac{3 + 3\kappa^2 + 4M^2\langle r_E^2\rangle}{48\pi M^3} = 0.97(6)\ \text{GeV}^{-3}$$

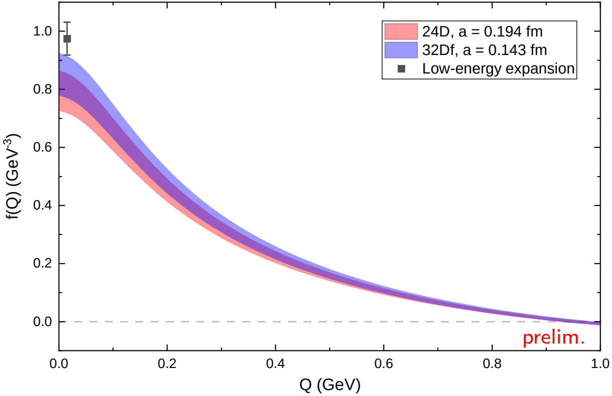
values are taken from PDG.

Preliminary result

- Lattice result of the integrand (connected diagrams only)

$$f(Q) = -\frac{\gamma(\tau_I)}{Q^2}[T_1(iQ, Q^2) - \lim_{Q\to 0} T_1(iQ, Q^2)]$$

same pion mass & volume, different lattice spacing



need further control systematics and add quark disconnected diagrams.

Outline

1. Background
2. Lattice QCD calculation of TPE to μH Lamb shift
(based on PRL 128 (2022) 17, 172002 + new progress)
3. Lattice QCD calculation of subtraction function
(ongoing)
4. Conclusion & Outlook

Conclusion & Outlook

- Two ways for better determining the TPE contribution:

- Direct LQCD calculation to full TPE.

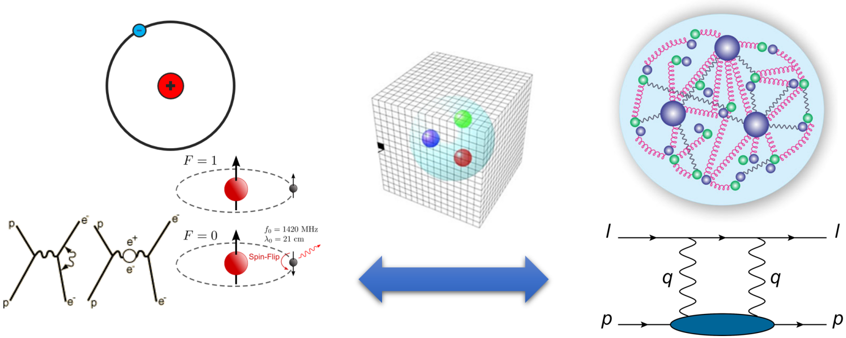
- Evaluate the subtraction function and combined with DR calculation.

- Future work:

- More statistics and better control the systematics.

- TPE correction to H & μH hyperfine splitting. (ongoing!)

- Also neutron TPE from LQCD.



- LQCD study of important quantities relevant for atomic spectroscopy

→ better understanding of hadron / nuclear structure, atomic physics, ⋯

Thank you!

further questions / discussions → fy_deg@pku.edu.cn